Processing and Validation of JEFF-3.1.2 Cross-section Library into Various Formats: ACE, PENDF, GENDF, MATXSR and BOXER

O. Cabellos[1, *]

[1] *Departamento de Ingenieria Nuclear, Universidad Politécnica de Madrid, 28006 Madrid, Spain*

Following the processing and validation of JEFF-3.1 performed in 2006 and presented in ND2007, and as a consequence of the latest updated of this library (JEFF-3.1.2) in February 2012, a new processing and validation of JEFF-3.1.2 cross section library is presented in this paper. The processed library in ACE format at ten different temperatures was generated with NJOY-99.364 nuclear data processing system. In addition, NJOY-99 inputs are provided to generate PENDF, GENDF, MATXSR and BOXER formats. The library has undergone strict QA procedures, being compared with other available libraries (e.g. ENDF/B-VII.1) and processing codes as PREPRO-2000 codes. A set of 119 criticality benchmark experiments taken from ICSBEP-2010 has been used for validation purposes.

I. INTRODUCTION

In February 2012, the JEFF-3.1.2 General Purpose Incident Neutron Library [1] was released which contains 115 updated material files since JEFF-3.1.1. This new release includes incident neutron data for 381 materials from ^{1}H to ^{255}Fm, including important light nuclei, structural materials, fission products, control rod materials and burnable poisons, all major and minor actinides. The nuclides to be processed are all of this evaluation and the JEFF-3.1.1 Scattering Thermal Library (STL).

The processing code system used was NJOY-99.364[3]. The NJOY-99 modules used in this processing are: MODER, RECONR, BROADR, HEATR, GASPR, PURR, ACER, GROUPR, MATXSR, ERRORR, COVR and VIEWR. To cover a large number of applications with MCNP, the library has been processed in ACE format at a wide range of temperatures: 293.6, 300, 400, 500, 600, 700, 800, 900, 1000, 1200 and 1800 Kelvins.

The PENDF library at 300K has been verified and compared to other available evaluated libraries (e.g. ENDF/B-VII.1 [2]) using JANIS-3.4[4], and comparison with other processing codes is performed with PREPRO-2000 code[5]. A Quality Assurance (QA) procedure [6] has been established to ensure the quality of the processed file. This QA procedure includes an expanded suite of 119 criticality benchmarks taken from the *International Criticality Safety Benchmark Evaluation Project-2010* (ICSBEP) [7] to assess the overall performance of JEFF-3.1.2. Results of the QA procedure are documented in a complete report distributed together with the ENDF and ACE files by NEA Data Bank.

* Corresponding author: oscar.cabellos@upm.es

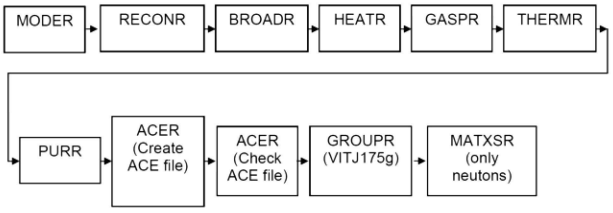

FIG. 1. NJOY sequence to process JEFF-3.1.2 in PENDF, ACE, GENDF and MATXSR formats.

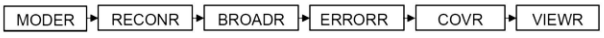

FIG. 2. NJOY sequence to process JEFF-3.1.2 covariance data in BOXER format.

II. PROCESSING EVALUATED NUCLEAR DATA INTO ACE, PENDF, GENDF, MATXSR AND BOXER FORMATS

NJOY-99 is a modular computer code used for converting evaluated nuclear data into different type of formats useful for criticality and shielding applications. The updated version NJOY-99.364 with some additional updates [8] is used in this work. The processing sequences used are shown in Figs. 1 and 2.

The ACE library contains continuous energy neutron cross section data files for use in the Monte Carlo code MCNP. Probability Tables (PT) have been generated for those materials containing unresolved resonance data. In addition, several JEFF-3.1.1 STL have been processed: hydrogen bound in polyethylene, water and ZrH; Graphite, D bound in D2O and Be.

Covariance data (MF31 to MF40) for materials in-

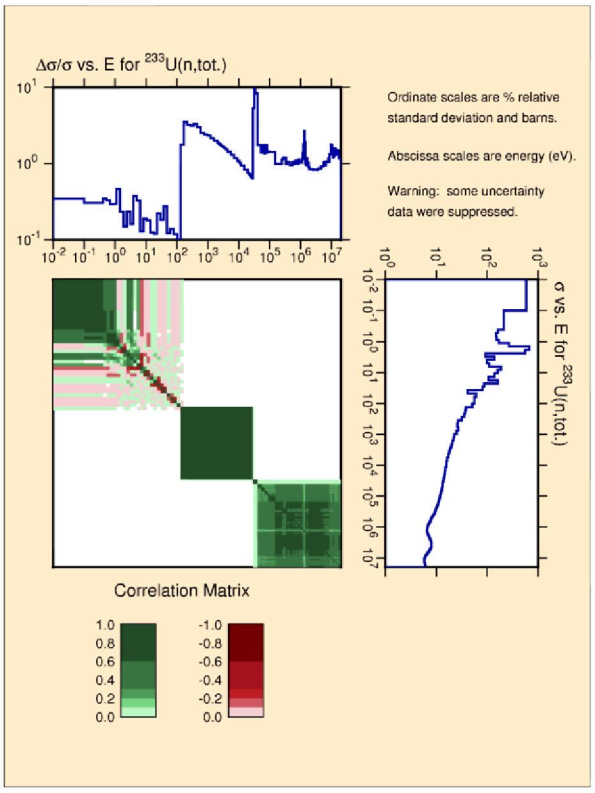

FIG. 3. Processing MF33- ^{233}U.

cluded in JEFF-3.1.2 has been processed using ERRORR/COVR modules. This work identified some isotopes (^{9}Be, ^{28}Si, ^{54}Fe, ^{233}U and ^{93}Nb) with problems in ENDF-6 format to process covariance data. Corrections for ^{233}U and ^{93}Nb were proposed and accepted to be included in the new JEFF-3.1.2 [8]. Fig. 3 shows processed covariance data for ^{233}U(n,tot).

III. QUALITY ASSURANCE PROCEDURE

A QA procedure for each JEFF-3.1.2 nuclide has been performed. The total number of messages from the NJOY-99 processing were compiled, all messages were understood and most of them were related to incomplete evaluations [6]. The reason to run the ACER module twice (see Fig. 1) is to evaluate the consistency of the ACE format where it is checked and problems are corrected. However, ACER does not include the capability to check the proper processing of the unresolved resonance probability tables [6]. PTs with negative cross section values cannot be allowed and the library file has to be recalculated without probability tables. JEFF-3.1.2 isotopes with negative PT values are listed as follows: ^{22}Na, ^{36}Ar, ^{95}Mo, ^{101}Ru, ^{105,110}Pd, ^{109}Ag, ^{141}Ce, ^{144,145,148}Nd, ^{144,147,152}Sm, ^{161}Dy, ^{185,187}Re, ^{235}U, ^{238}Np, ^{240,243}Pu, ^{241}Am, ^{250,251,252}Cf and ^{253}Es. It is necessary to make

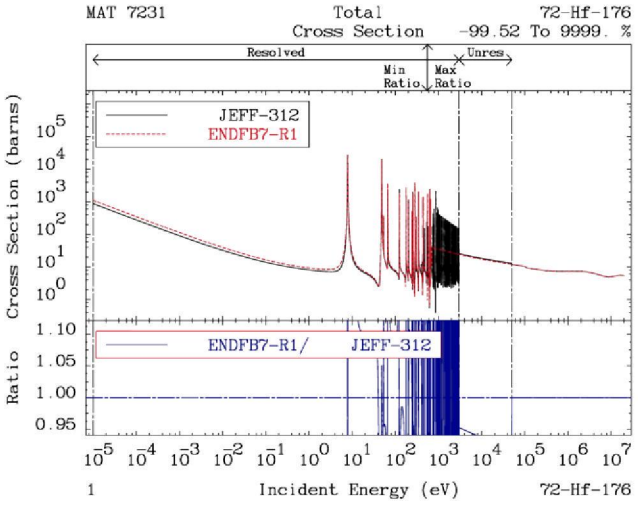

FIG. 4. Comparison of ^{176}Hf(n,tot) between JEFF-3.1.2 and END/B-VII.1 as it is shown with COMPLOT [5] program.

a special mention to the case of PTs for ^{238}Pu, where problems have been found running MCNP5 [9].

QA procedure developed in Ref. [10] has been applied, checking the contents of all the ACE-formatted files, being converted back to ENDF-6 format using the code ACELST[11]. These ENDF-6 files were compared with the original evaluation using both NJOY-99 and PREPRO-2010 code[5] (LINEAR + RECENT + SIGMA1). Warnings and messages from PREPRO-2010 codes are useful to complete an additional checking. A comparison between JEFF-3.1.2 and ENDF/B-VII.1 is also performed (see an example in Fig. 4). Finally, INTER [12] and NJOY-99/BROADR calculations at 293.6K are used to compare integral data with other evaluations.

A. Criticality Validation

An expanded criticality validation suite taken from the ICSBEP [7], and presented in Ref. [13] is used to assess JEFF-3.1.2 in criticality calculation. This Benchmark suite contains 119 criticality cases, and it provides a general indication of the overall performance of a nuclear data library [13]. In TABLE I, Benchmark cases with differences larger than two times the experimental standard deviation using JEFF-3.1.2 are shown.

Regarding JEFF-3.1.2, it can be observed: i) deficiencies in fast cases (PU, ^{233}U, HEU and IEU) and intermediate cases (HEU and IEU), ii) cross sections for ^{239}Pu should be re-examined in the thermal range (pu-sol-therm-009-case3a), and iii) good agreement for LEU cases are shown.

For ^{233}U, ENDF/B-VII.1 gives a better agreement than JEFF-3.1.2, whereas for the rest of the cases a similar behaviour between both libraries is shown.

TABLE I. Summary of a MCNP Criticality Validation Suite with differences larger than two times the experimental standard deviation.

	Spectrum	Moderator/Reflector	Benchmark name	Benchmark	ENDF/B-VII.1b3[13]	JEFF-3.1.2
U233	Fast	Unreflected	u233-met-fast-001	1.0000 ± 0.0010	0.9995 ± 0.0003	*1.0045 ± 0.0003*
		HEU	u233-met-fast-002-CASE_2	1.0000 ± 0.0011	1.0006 ± 0.0003	*1.0032 ± 0.0003*
		Normal Uranium	u233-met-fast-003-CASE_1	1.0000 ± 0.0010	0.9996 ± 0.0003	*1.0051 ± 0.0003*
			u233-met-fast-003-CASE_2	1.0000 ± 0.0010	1.0001 ± 0.0003	*1.0049 ± 0.0003*
			u233-met-fast-006	1.0000 ± 0.0014	0.9995 ± 0.0003	*1.0058 ± 0.0003*
		Tungsten	u233-met-fast-004-CASE_1	1.0000 ± 0.0007	*1.0049 ± 0.0003*	*1.0055 ± 0.0003*
			u233-met-fast-004-CASE_2	1.0000 ± 0.0008	*1.0052 ± 0.0003*	*1.0037 ± 0.0003*
HEU	Fast	Unreflected	heu-met-fast-001	1.0000 ± 0.0010	0.9994 ± 0.0003	*0.9965 ± 0.0003*
			heu-met-fast-008	0.9989 ± 0.0016	*0.9957 ± 0.0003*	*0.9923 ± 0.0003*
		Steel	heu-met-fast-013	0.9990 ± 0.0015	*0.9975 ± 0.0003*	*0.9914 ± 0.0003*
		Beryllium	heu-met-fast-009-case1	0.9992 ± 0.0015	*0.9949 ± 0.0003*	*0.9932 ± 0.0003*
		Water	heu-met-fast-004-case1	1.0020 ± 0.0010	1.0028 ± 0.0003	*0.9951 ± 0.0003*
		Unreflected	heu-met-fast-015	0.9996 ± 0.0017	*0.9943 ± 0.0003*	*0.9902 ± 0.0003*
		Paraffin	heu-met-fast-026-case9	1.0000 ± 0.0038	*1.0037 ± 0.0003*	*0.9871 ± 0.0003*
	Intermediate	Graphite, copper	heu-met-inter-006-case1	0.9977 ± 0.0008	*0.9930 ± 0.0004*	*0.9929 ± 0.0003*
			heu-met-inter-006-case2	0.9997 ± 0.0008	*0.9960 ± 0.0004*	*0.9946 ± 0.0004*
			heu-met-inter-006-case3	1.0015 ± 0.0009	*1.0006 ± 0.0004*	*0.9980 ± 0.0003*
			heu-met-inter-006-case4	1.0016 ± 0.0008	*1.0075 ± 0.0003*	*1.0050 ± 0.0003*
IEU	Fast	Duralumin	ieu-met-fast-006-case2	1.0000 ± 0.0023	*0.9957 ± 0.0003*	*0.9922 ± 0.0003*
		Unreflected	ieu-met-fast-001-case3	0.9993 ± 0.0005	*1.0014 ± 0.0003*	*0.9972 ± 0.0003*
		Unreflected	ieu-met-fast-001-case4	1.0002 ± 0.0005	*1.0015 ± 0.0003*	*0.9973 ± 0.0003*
		Depleted U	ieu-met-fast-007-case1	1.0049 ± 0.0008	1.0049 ± 0.0002	*0.9984 ± 0.0002*
	Intermediate	Normal U, steel	mix-met-fast-008-case7	1.0030 ± 0.0025	*1.0193 ± 0.0002*	*1.0170 ± 0.0002*
PU	Fast	Thorium	pu-met-fast-008-case2	1.0000 ± 0.0006	*0.9977 ± 0.0003*	*1.0023 ± 0.0003*
		Tungsten	pu-met-fast-005-CASE_1	1.0000 ± 0.0013	*1.0093 ± 0.0003*	*1.0038 ± 0.0003*
		Water	pu-met-fast-011-CASE_1	1.0000 ± 0.0010	1.0002 ± 0.0003	*0.9974 ± 0.0003*
	Thermal	Unreflected	pu-sol-therm-009-case3a	1.0000 ± 0.0033	*1.0190 ± 0.0002*	*1.0145 ± 0.0002*

IV. CONCLUSION

JEFF-3.1.2 library has been processed in different formats: PENDF, GENDF, MATXSR, BOXER, and in ACE format at ten different temperatures for a wide range of MCNP applications. QA procedures have been applied to guarantee the quality of the JEFF-3.1.2 processed file. The processed data were judged to be acceptable according to an extensive QA procedure: i) checking ACE files, ii) compiling warnings and messages from NJOY-99 and PREPRO-2010, iii) using an expanded suite of 119 criticality benchmarks providing a general indication of the overall performance of JEFF-3.1.2 nuclear data library. The ENDF library, processed library, NJOY inputs and the documentation associated are distributed by NEA Data Bank upon request.

Acknowledgements: This work was supported by the OECD/Nuclear Energy Agency (NEA) Data Bank.

[1] A.J. Koning, E. Bauge, C.J. Dean *et al.*, J. Korean Phys. Soc. **59**, 1057 (2011).
[2] M.B. Chadwick *et al.* Nucl. Data Sheets **112**, 2887 (2011).
[3] "NJOY 99 Nuclear Data Processing System", `http://t2.lanl.gov/codes/njoy99/`, (2011).
[4] JANIS-3.4, `http://www.oecd-nea.org/janis/`, (2012).
[5] D.E. Cullen, PREPRO 2010, IAEA-NDS-39, Rev. 14 (2010).
[6] O. Cabellos, EDP Sciences, 697 (2008).
[7] International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP), OECD/NEA, NEA/NSC/DOC(95)03, Paris (2011).
[8] O. Cabellos, JEFF/DOC-1436 (2012).
[9] Los Alamos National Laboratory, April 24, 2003. MCNP-A General Monte Carlo N-Particle Transport Code, Version 5.
[10] D. Lopez Aldama, A. Trkov, ADS-Lib/V1.0, IAEA (2005).
[11] A. Trkov, Private communication on ACELST code (2002).
[12] "Program INTER, ENDF-6 Checking & Utility Codes", Available from (`http://www-nds.iaea.org/public/endf/utility/`).
[13] R.D. Mosteller, F.B. Brown, B.C. Kiedrowski, Report LA-UR- 11-00240 (2011).